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Top Down General Ionization Formula

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The general formula for ionization energy derives from the **energy minimizing** generating function given in Equation (10.449)

$$\Phi(r,\theta,\phi)=\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}B_{\ell,m}r^{-(\ell+1)}Y_\ell^m(\theta,\phi)$$

Generating function Equation (I.22):

$$Y_{lm}(\theta,\phi)=\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}P_l^m(\cos\theta)e^{im\phi}$$

The Associated Legendre Polynomial generating function:

$$P_l^m(x)=(-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x)$$
$$=\frac{(-1)^m}{2^l\,l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l,$$

Generating function Equation (2.38) for B[ℓ,m]:

$$\mathbf{B}=\sum_{\ell,m}\left[a_E(\ell,m)f_\ell(kr)\mathbf{X}_{\ell,m}-\frac{i}{k}a_M(\ell,m)\nabla\times g_\ell(kr)\mathbf{X}_{\ell,m}\right]$$

Generating function Equation (2.39) -- also applicable to $f[\ell]$:

$$g_\ell(kr)=A_\ell^{(1)}h_\ell^{(1)}+A_\ell^{(2)}h_\ell^{(2)}$$

Generating function Equation (2.40):

$$\mathbf{X}_{\ell,m}(\theta,\phi)=\frac{1}{\sqrt{\ell(\ell+1)}}\mathbf{L}Y_{\ell,m}(\theta,\phi)$$

Equation (2.41):

$$\mathbf{L}=\frac{1}{i}(\mathbf{r}\times\nabla)$$

Generating function Equation (2.42):

$$a_E(\ell,m)=\frac{4\pi k^2}{i\sqrt{\ell(\ell+1)}}\int Y_\ell^{m*}\left\{\rho\frac{\partial}{\partial r}\left[rj_\ell(kr)\right]+\frac{ik}{c}(\mathbf{r}\cdot\mathbf{J})j_\ell(kr)-ik\nabla\cdot(r\times\boldsymbol{M})j_\ell(kr)\right\}d^3x$$

Generating function Equation (2.43):

$$a_M(\ell,m) = \frac{-4\pi k^2}{\sqrt{\ell(\ell+1)}} \int j_\ell(kr) Y_\ell^{m*} \mathbf{L} \cdot \left(\frac{\mathbf{J}}{c} + \nabla \times \boldsymbol{M} \right) d^3x$$

Generating function Equation (2.44):

$$\begin{aligned}
\mathbf{J} &= \frac{m\omega_n}{2\pi} \frac{e}{4\pi r_n^2} N[\delta(r-r_n)] \mathrm{Re}\left\{ Y_\ell^m(\theta,\phi) \right\} \left[\mathbf{u}(t) \times \mathbf{r} \right] \\
&= \frac{m\omega_n}{2\pi} \frac{e}{4\pi r_n^2} N'[\delta(r-r_n)] \left(P_\ell^m(\cos\theta) \cos(m\phi + m\omega_n t) \right) [\mathbf{u} \times \mathbf{r}] \\
&= \frac{m\omega_n}{2\pi} \frac{e}{4\pi r_n^2} N'[\delta(r-r_n)] \left(P_\ell^m(\cos\theta) \cos(m\phi + m\omega_n t) \right) \sin\theta \hat{\phi}
\end{aligned}$$

Equation (2.45):

$$\hat{\phi} = \frac{\hat{u} \times \hat{r}}{|\hat{u} \times \hat{r}|} = \frac{\hat{u} \times \hat{r}}{\sin\theta}; \qquad \hat{u} = \hat{z} = orbital\ axis$$

Equation (2.46):

$$\hat{\theta} = \hat{\phi} \times \hat{r}$$

Condition given for the degenerate Equation (2.47):

$$\mathbf{r} \cdot \mathbf{J} = 0$$

Condition given for "lightlike *k*"...

$$k = \omega_n / c$$

...showing "*There is no radiation*."

Remaining symbols to be defined and their occurrence:

N' in the final form of (2.44),
j[ℓ], m* and M in (2.42) and (2.43)
A and h in (2.39)